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Thermodynamic limit and surface energy of the *XXZ* spin chain with arbitrary boundary fields

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Abstract

In two previous papers [26,27], the exact solutions of the spin-$\frac{1}{2}$ chains with arbitrary boundary fields were constructed via the off-diagonal Bethe ansatz (ODBA). Here we introduce a method to approach the thermodynamic limit of those models. The key point is that at a sequence of degenerate points of the crossing parameter $\eta = \eta_m$, the off-diagonal Bethe ansatz equations (BAEs) can be reduced to the conventional ones. This allows us to extrapolate the formulae derived from the reduced BAEs to arbitrary η case with $O(N^{-2})$ corrections in the thermodynamic limit $N \to \infty$. As an example, the surface energy of the *XXZ* spin chain model with arbitrary boundary magnetic fields is derived exactly. This approach can be generalized to all the ODBA solvable models.

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1. Introduction

The integrable models have played very important roles in statistical physics [1], quantum field theory [2] and low-dimensional condensed matter physics [3,4]. In the recent years, new applications have been found on cold atom systems and AdS/CFT correspondence. For examples, the Lieb–Liniger model [5,6], Yang model [7] and the one-dimensional Hubbard model [8] have provided important benchmarks for the one-dimensional cold atom systems and even fitted experimental data with incredibly high accuracy [9]. On the other hand, the anomalous dimensions of single-trace operators of $\mathcal{N} = 4$ super-symmetric Yang–Mills (SYM) field theory can be given by the eigenvalues of certain closed integrable spin chains [10,11] while the anomalous dimensions of the determinant-like operators of $\mathcal{N} = 4$ SYM [12,13] can be mapped to the eigenvalue problem of certain open integrable spin chains with boundary fields [14,15,11]. By AdS/CFT correspondence the boundaries correspond to open strings attached to maximal giant gravitons [16,13]. Sometimes those boundaries may even break the $U(1)$ symmetry.

Indeed, among the family of quantum integrable models, there exists a large class of models which do not possess $U(1)$ symmetry and make the conventional Bethe ansatz methods such as coordinate Bethe ansatz [17,18], algebraic Bethe ansatz [19,20] and T–Q relation [21,22] quite hard to be used because of lacking a proper reference state. Some famous examples are the *XYZ* spin chain with odd number of sites [23], the anisotropic spin torus [24,25] and the quantum spin chains with non-diagonal boundary fields [26–29]. Those models have been realized also possessing important applications in non-equilibrium statistical physics (e.g., stochastic processes [30–32]), in condensed matter physics (e.g., a Josephson junction embedded in a Luttinger liquid [33], spin–orbit coupling systems, one-dimensional cold atoms coupled with a BEC reservoir etc.) and in high energy physics (e.g., open strings and coupled D-branes). Very recently, a systematic method for solving the integrable models without $U(1)$ symmetry, i.e., the so-called off-diagonal Bethe ansatz (ODBA) method, was proposed [25–27] and several long-standing models were solved exactly [25–27,34–37]. However, an important issue about this kind of models, i.e., the thermodynamic limit, is still open. The difficulty to approach the thermodynamic limit of those models lies in that there is an off-diagonal term (or inhomogeneous term) in the Bethe ansatz equations (BAEs), which makes the distributions of the Bethe roots quite opaque.

In this paper, we propose that the thermodynamic limit of the ODBA solvable models for arbitrary crossing parameter η can be derived from those at a sequence of degenerate points $\eta = \eta_m$ up to the order $O(N^{-2})$. At these special points, the ODBA equations are reduced to the usual BAEs which allow us to use the usual tools to derive the thermodynamic quantities. As $\eta_{m+1} - \eta_m = 2i\pi/N$, those degenerate points become dense in the thermodynamic limit $N \to \infty$. In the following text, we take the *XXZ* spin chain model with arbitrary boundary fields as an example to elucidate how the method works.

The paper is organized as follows: In the next section, the Hamiltonian and the associated ODBA equations are introduced. Section 3 is attributed to the calculation of the surface energy at the degenerate points $\eta = \eta_m$. The analysis about arbitrary η case is given in Section 4. Concluding remarks and discussions are given in Section 5.

2. The model and its ODBA solutions

Let us consider a typical ODBA solvable model, i.e., the *XXZ* spin chain with arbitrary boundary fields. The Hamiltonian reads

$$H=\sum_{j=1}^{N-1}\left[\sigma_j^x\sigma_{j+1}^x+\sigma_j^y\sigma_{j+1}^y+\cosh\eta\sigma_j^z\sigma_{j+1}^z\right]+\vec{h}_-\cdot\vec{\sigma}_1+\vec{h}_+\cdot\vec{\sigma}_N, \tag{2.1}$$

where σ_j^α ($\alpha=x,y,z$) are the Pauli matrices as usual and $\vec{h}_\pm=(h_\pm^x,h_\pm^y,h_\pm^z)$ are the boundary magnetic fields. For convenience, we adopt the notations in Ref. [27] to parameterize the boundary fields as

$$\begin{aligned}&h_\pm^x=\frac{\sinh\eta\cosh\theta_\pm}{\sinh\alpha_\pm\cosh\beta_\pm},\qquad h_\pm^y=\frac{i\sinh\eta\sinh\theta_\pm}{\sinh\alpha_\pm\cosh\beta_\pm},\\&h_\pm^z=\mp\sinh\eta\coth\alpha_\pm\tanh\beta_\pm.\end{aligned} \tag{2.2}$$

The eigenvalues of the Hamiltonian thus read

$$\begin{aligned}E=-\sinh\eta\Bigg[&\coth(\alpha_-)+\tanh(\beta_-)+\coth(\alpha_+)+\tanh(\beta_+)\\&+2\sum_{j=1}^{M}\coth(\mu_j+\eta)-(N-1)\coth\eta\Bigg],\end{aligned} \tag{2.3}$$

where the Bethe roots μ_j are determined by the ODBA equations

$$\begin{aligned}&\frac{\bar{c}\sinh(2\mu_j+\eta)\sinh(2\mu_j+2\eta)}{2\sinh(\mu_j+\alpha_-+\eta)\cosh(\mu_j+\beta_-+\eta)}\frac{\sinh^n\mu_j\sinh^{M+N}(\mu_j+\eta)}{\sinh(\mu_j+\alpha_++\eta)\cosh(\mu_j+\beta_++\eta)}\\&\quad=\prod_{l=1}^{M}\sinh(\mu_j+\mu_l+\eta)\sinh(\mu_j+\mu_l+2\eta),\end{aligned} \tag{2.4}$$

$j=1,\ldots,M$, and

$$\bar{c}=\cosh\left[(N+2n+1)\eta+\alpha_-+\beta_-+\alpha_++\beta_++2\sum_{j=1}^{M}\mu_j\right]-\cosh(\theta_--\theta_+), \tag{2.5}$$

with n a non-negative even (odd) integer[1] for even (odd) N and $M=N+n$. Interestingly, when the boundary parameters and the crossing parameter η satisfy the following constraint condition [27,38]

$$(2M_1-N+1)\eta+\alpha_-+\beta_-+\alpha_++\beta_+\pm(\theta_--\theta_+)=2\pi im, \tag{2.6}$$

there does exist a solution to (2.4)–(2.5) such that the parameter $\bar{c}=0$ and hence the Bethe roots are classified into two types of pairs

$$(\mu_l,-\mu_l-\eta),\qquad(\mu_l,-\mu_l-2\eta),$$

with M_1 the number of the first pairs and m an arbitrary integer.

Let us focus on the gapless region, i.e., imaginary η and $\theta_\pm$ case. Without losing generality, we put $\alpha_\pm$ imaginary and $\beta_\pm$ real to ensure the boundary fields being real. Let us examine the

[1] In Ref. [27], $n=0$ for even N and $n=1$ for odd N were adopted. The T–Q relation with arbitrary n was considered in Ref. [26].

Table 1
The numerical solutions of (2.8) for $N=3$ with the parameters $\eta=-i$, $\alpha_+=2i$, $\alpha_-=3i$, $\beta_+=1$, $\beta_-=-1$, $\theta_+=2i$, $\theta_-=i$. el indicates the number of the energy levels.

μ_1	μ_2	μ_3	E	el
$-1.48510+0.67075i$	$-1.48510+2.47085i$	$0.36994-0.00000i$	-9.10664	1
$-0.63430-1.57080i$	$-0.38556+0.50089i$	$-0.38556-0.50089i$	-5.80407	2
$-1.11069+1.00247i$	$-1.11069+2.13912i$	$-1.10123-0.00000i$	-5.30177	3
$-1.68396-0.65365i$	$0.59457+1.57080i$	$1.68396-0.65365i$	-4.08354	4
$-0.51260-1.57080i$	$-0.38055+0.00000i$	$-0.00000+0.64158i$	3.46000	5
$-1.56515-0.66501i$	$-0.00000+0.64158i$	$1.56515-0.66501i$	5.73191	6
$-0.00000+0.64159i$	$0.25391-1.57080i$	$1.09544+0.00000i$	6.81205	7
$-0.94157+1.57080i$	$-0.00000+0.64159i$	$0.20977+1.57080i$	8.29206	8

solutions at the degenerate points $\eta=\eta_m$ (corresponding to the case of $\bar{c}=0$ and $M_1=N$) and $\beta_\pm=\pm\beta$,

$$\eta_m=-\frac{\alpha_-+\alpha_+\pm(\theta_--\theta_+)+2\pi i m}{N+1}. \tag{2.7}$$

For convenience, let us take $\lambda_j=\mu_j+\frac{\eta}{2}$, $ia_\pm=\alpha_\pm+\frac{\eta}{2}$, $\eta=i\theta$, with $a_\pm,\theta\in(0,\pi)$. With these parameters, the reduced BAEs for $\eta=\eta_m$ become[2]

$$\begin{aligned}&\left[\frac{\sinh(\lambda_j-i\frac{\theta}{2})}{\sinh(\lambda_j+i\frac{\theta}{2})}\right]^{2N}\frac{\sinh(2\lambda_j-i\theta)}{\sinh(2\lambda_j+i\theta)}\frac{\sinh(\lambda_j+ia_+)}{\sinh(\lambda_j-ia_+)}\\&\quad\times\frac{\sinh(\lambda_j+ia_-)}{\sinh(\lambda_j-ia_-)}\frac{\cosh(\lambda_j+\beta+i\frac{\theta}{2})}{\cosh(\lambda_j+\beta-i\frac{\theta}{2})}\frac{\cosh(\lambda_j-\beta+i\frac{\theta}{2})}{\cosh(\lambda_j-\beta-i\frac{\theta}{2})}\\&\quad=-\prod_{l=1}^{N}\frac{\sinh(\lambda_j-\lambda_l-i\theta)\sinh(\lambda_j+\lambda_l-i\theta)}{\sinh(\lambda_j-\lambda_l+i\theta)\sinh(\lambda_j+\lambda_l+i\theta)},\end{aligned} \tag{2.8}$$

where $j=1,\dots,N$. The above reduced BAEs were firstly observed in [38]. The corresponding eigenenergy is given by

$$\begin{aligned}E=&-\sum_{j=1}^{N}\frac{4\sin^2\theta}{\cosh(2\lambda_j)-\cos\theta}-\sin\theta\big[\cot(a_+-\theta/2)+\cot(a_--\theta/2)\big]\\&+(N-1)\cos\theta.\end{aligned} \tag{2.9}$$

We confirm that for $\eta=\eta_m$, the reduced BAEs (2.8) give a complete set of solutions as verified numerically [39]. Here, we have checked this statement numerically for small N. The numerical solutions of (2.8) for $N=3,4$ with randomly chosen boundary parameters are shown in Tables 1 and 2, respectively. The eigenvalues E of the Hamiltonian shown in the tables are exactly the same as those from exact diagonalization.

3. The surface energy for $\eta=\eta_m$

Let us consider the ground state energy at the degenerate crossing parameter points given by (2.7). Since a real λ_j contributes negative energy, the Bethe roots should fill the real axis as

[2] The reduced BAEs were derived from the regularity of the reduced $\Lambda(u)$ in [27]. See also [38].

Table 2
The numerical solutions of (2.8) for $N = 4$ with the parameters $\theta = 1$, $a_+ = 2.5$, $a_- = 1.5$, $\beta = 1$, $\theta_- = 3i$, $\theta_+ = -5i$, $m = 0$.

λ_1	λ_2	λ_3	λ_4	E	*el*
$-1.66762 - 0.00000i$	$-1.21632 + 1.57080i$	$-0.55018 + 0.00000i$	$-0.21316 + 0.00000i$	-5.93342	1
$-0.92025 - 0.00000i$	$-0.91893 + 0.99518i$	$0.20501 - 3.14159i$	$0.91893 + 0.99518i$	-3.85243	2
$-0.94690 - 2.65582i$	$-0.68831 - 1.57080i$	$-0.19733 - 0.00000i$	$0.94690 + 3.62737i$	-3.58123	3
$-0.46931 - 1.57080i$	$-0.17931 - 0.00000i$	$1.43232 + 1.57080i$	$1.90426 - 0.00000i$	-2.35148	4
$-0.91410 + 0.00000i$	$-0.91160 - 0.99287i$	$-0.91160 + 0.99287i$	$-0.50119 + 0.00000i$	-1.47531	5
$-0.87562 - 3.62850i$	$-0.87562 + 0.48690i$	$-0.57755 - 1.57080i$	$-0.45893 - 0.00000i$	-1.36888	6
$0.39497 - 3.14159i$	$0.39554 + 1.57080i$	$1.40894 + 1.57080i$	$1.87940 + 0.00000i$	-0.43122	7
$-1.77682 + 0.00000i$	$-0.48316 + 0.50058i$	$0.48316 + 0.50058i$	$1.32868 - 1.57080i$	0.08195	8
$-1.40329 + 0.00000i$	$-0.89579 - 2.13792i$	$0.89236 + 0.00000i$	$0.89579 + 1.00367i$	0.98414	9
$-0.55149 + 0.49964i$	$-0.38646 - 1.57080i$	$0.55149 + 0.49964i$	$1.39986 + 0.00000i$	1.15594	10
$-1.80115 - 0.00000i$	$-1.32916 + 1.57080i$	$-0.72884 - 0.00000i$	$-0.28785 + 1.57080i$	1.68692	11
$-0.92875 - 1.57080i$	$-0.90786 + 0.99956i$	$-0.90786 + 2.14204i$	$-0.90693 + 0.00000i$	2.08877	12
$-0.86225 + 1.57080i$	$-0.46738 - 2.64162i$	$0.33674 - 1.57080i$	$0.46738 + 0.49997i$	2.26194	13
$-0.93579 + 0.99864i$	$-0.93536 - 0.00000i$	$0.23087 + 1.57080i$	$0.93579 - 2.14295i$	3.06940	14
$0.22280 + 1.57080i$	$0.92385 - 1.57080i$	$1.13160 - 0.48933i$	$1.13160 + 0.48933i$	3.33186	15
$-1.56849 - 1.57080i$	$-0.75387 + 1.57080i$	$0.19162 + 1.57080i$	$2.05390 + 0.00000i$	4.33306	16

long as possible. However, in the thermodynamic limit, the maximum number of Bethe roots accommodated by the real axis is only about $N/2$, some of the roots must be repelled to the complex plane and form a string [40]. Suppose there is a k string[3] in the ground state configuration with

$$\lambda_l^s = \lambda^r + i\frac{\theta}{2}(k + 1 - 2l) + O\big(e^{-\delta N}\big), \quad l = 1, \ldots, k, \tag{3.1}$$

where λ^r is the position of the string on the real axis and δ is a positive number to account for the small deviation. Substituting (3.1) into (2.8) and omitting the exponentially small corrections we obtain

$$\begin{aligned}
&\left[\frac{\sinh(\lambda_j - i\frac{\theta}{2})}{\sinh(\lambda_j + i\frac{\theta}{2})}\right]^{2N} \frac{\sinh(2\lambda_j - i\theta)}{\sinh(2\lambda_j + i\theta)} \frac{\sinh(\lambda_j + ia_+)}{\sinh(\lambda_j - ia_+)} \\
&\quad \times \frac{\sinh(\lambda_j + ia_-)}{\sinh(\lambda_j - ia_-)} \frac{\cosh(\lambda_j + \beta + i\frac{\theta}{2})}{\cosh(\lambda_j + \beta - i\frac{\theta}{2})} \frac{\cosh(\lambda_j - \beta + i\frac{\theta}{2})}{\cosh(\lambda_j - \beta - i\frac{\theta}{2})} \\
&= -\prod_{l=1}^{N-k} \frac{\sinh(\lambda_j - \lambda_l - i\theta)\sinh(\lambda_j + \lambda_l - i\theta)}{\sinh(\lambda_j - \lambda_l + i\theta)\sinh(\lambda_j + \lambda_l + i\theta)} \\
&\quad \times \frac{\sinh(\lambda_j + \lambda^r - i\frac{\theta}{2}(k+1))\sinh(\lambda_j + \lambda^r - i\frac{\theta}{2}(k-1))}{\sinh(\lambda_j + \lambda^r + i\frac{\theta}{2}(k+1))\sinh(\lambda_j + \lambda^r + i\frac{\theta}{2}(k-1))} \\
&\quad \times \frac{\sinh(\lambda_j - \lambda^r - i\frac{\theta}{2}(k+1))\sinh(\lambda_j - \lambda^r - i\frac{\theta}{2}(k-1))}{\sinh(\lambda_j - \lambda^r + i\frac{\theta}{2}(k+1))\sinh(\lambda_j - \lambda^r + i\frac{\theta}{2}(k-1))},
\end{aligned} \tag{3.2}$$

where $j = 1, \ldots, N - k$.

[3] Another type of strings may exist in this model. Different choice of the bulk string does not affect the surface energy as the string's contribution to the ground state energy is zero in the thermodynamic limit. For rational π/η, there is a constraint for k. Here we consider the case of π/η_m away from those special values. In fact we can always take N a prime number to ensure the possible k being large enough. For detail, see [40].

We consider the $a_\pm \in (\frac{\pi}{2}, \pi)$ case. Taking the logarithm of (3.2) we have

$$\begin{aligned}
&\phi_1(\lambda_j) + \frac{1}{2N}\big[\phi_2(2\lambda_j) - \phi_{2a_+/\theta}(\lambda_j) - \phi_{2a_-/\theta}(\lambda_j) + B(\lambda_j+\beta) + B(\lambda_j-\beta) \\
&\qquad - \pi - \phi_{k+1}\big(\lambda_j-\lambda^r\big) - \phi_{k-1}\big(\lambda_j-\lambda^r\big) - \phi_{k+1}\big(\lambda_j+\lambda^r\big) - \phi_{k-1}\big(\lambda_j+\lambda^r\big)\big] \\
&\quad = 2\pi\frac{I_j}{2N} + \frac{1}{2N}\sum_{l=1}^{N-k}\big[\phi_2(\lambda_j-\lambda_l) + \phi_2(\lambda_j+\lambda_l)\big],
\end{aligned} \tag{3.3}$$

where I_j is an integer and

$$\begin{aligned}
\phi_m(\lambda_j) &= -i\ln\frac{\sinh(\lambda_j - i\frac{m\theta}{2})}{\sinh(\lambda_j + i\frac{m\theta}{2})} \\
B(\lambda_j) &= -i\ln\frac{\cosh(\lambda_j + i\frac{\theta}{2})}{\cosh(\lambda_j - i\frac{\theta}{2})}.
\end{aligned} \tag{3.4}$$

For convenience, let us put $\lambda_l = -\lambda_{-l}$ and define the counting function $Z(\lambda)$ as

$$\begin{aligned}
Z(\lambda) = \frac{1}{2\pi}\Bigg\{&\phi_1(\lambda) + \frac{1}{2N}\Bigg[\phi_2(2\lambda) - \phi_{2a_+/\theta}(\lambda) - \phi_{2a_-/\theta}(\lambda) + B(\lambda+\beta) \\
&+ B(\lambda-\beta) - \phi_{k+1}\big(\lambda-\lambda^r\big) - \phi_{k-1}\big(\lambda-\lambda^r\big) - \phi_{k+1}\big(\lambda+\lambda^r\big) \\
&- \phi_{k-1}\big(\lambda+\lambda^r\big) - \pi - \sum_{l=1}^{N-k}\big[\phi_2(\lambda-\lambda_l) + \phi_2(\lambda+\lambda_l)\big]\Bigg]\Bigg\}.
\end{aligned} \tag{3.5}$$

Obviously, $Z(\lambda_j) = I_j/2N$ coincides with Eq. (3.3). In the thermodynamic limit $N \to \infty$, the density of the real roots $\rho(\lambda)$ is

$$\begin{aligned}
\rho(\lambda) &= \frac{dZ(\lambda)}{d\lambda} - \frac{1}{2N}\delta(\lambda) \\
&= a_1(\lambda) + \frac{1}{2N}\big[2a_2(2\lambda) - a_{2a_+/\theta}(\lambda) - a_{2a_-/\theta}(\lambda) + b(\lambda+\beta) + b(\lambda-\beta) \\
&\quad - a_{k+1}\big(\lambda-\lambda^r\big) - a_{k-1}\big(\lambda-\lambda^r\big) - a_{k+1}\big(\lambda+\lambda^r\big) - a_{k-1}\big(\lambda+\lambda^r\big) \\
&\quad - \delta(\lambda)\big] - \int_{-\infty}^{\infty} a_2(\lambda-\nu)\rho(\nu)d\nu,
\end{aligned} \tag{3.6}$$

with

$$a_m(\lambda) = \frac{1}{2\pi}\frac{d\phi_m(\lambda)}{d\lambda} = \frac{1}{\pi}\frac{\sin m\theta}{\cosh 2\lambda - \cos m\theta}, \tag{3.7}$$

$$b(\lambda) = \frac{1}{2\pi}\frac{dB(\lambda)}{d\lambda} = \frac{1}{\pi}\frac{\sin\theta}{\cosh(2\lambda) + \cos\theta}, \tag{3.8}$$

where the $\delta(\lambda)$ term accounts for the hole at $\lambda = 0$ which is a solution of the BAEs but can never be occupied in any case. With the Fourier transformations

$$\hat{f}(\omega) = \int_{-\infty}^{\infty} f(\lambda)e^{i\omega\lambda}d\lambda,$$

we obtain

$$\hat{\rho}(\omega) = \hat{\rho}_0(\omega) + \hat{\rho}_b(\omega), \tag{3.9}$$

where

$$\hat{\rho}_0(\omega) = \frac{\hat{a}_1(\omega)}{1 + \hat{a}_2(\omega)}, \tag{3.10}$$

$$\begin{aligned}\hat{\rho}_b(\omega) = {} & \frac{1}{2N[1 + \hat{a}_2(\omega)]}\left\{\hat{a}_2\left(\frac{\omega}{2}\right) - \hat{a}_{2a_+/\theta}(\omega) - \hat{a}_{2a_-/\theta}(\omega) + 2\cos(\beta\omega)\hat{b}(\omega)\right. \\ & \left. - 2\cos\bigl(\lambda^r\omega\bigr)\bigl[\hat{a}_{k+1}(\omega) + \hat{a}_{k-1}(\omega)\bigr] - 1\right\},\end{aligned} \tag{3.11}$$

$$\hat{a}_m(\omega) = \frac{\sinh(\pi\omega/2 - \delta_m\pi\omega)}{\sinh(\pi\omega/2)}, \qquad \hat{b}(\omega) = \frac{\sinh(\theta\omega/2)}{\sinh(\pi\omega/2)}, \tag{3.12}$$

with $\delta_m \equiv \frac{m\theta}{2\pi} - \lfloor\frac{m\theta}{2\pi}\rfloor$ denoting the fraction part of $\frac{m\theta}{2\pi}$. For $\rho(\lambda)$ is the density of the real roots and $M_1 = N$, the following equation must hold

$$N\int_{-\infty}^{\infty}\rho(\lambda)d\lambda + k = N, \tag{3.13}$$

which gives the length of the string k,

$$k = \frac{N}{2} - \frac{a_+ + a_- + 2\pi(\delta_{k+1} + \delta_{k-1}) - 3\pi}{2(\pi - \theta)}. \tag{3.14}$$

Obviously, k has the order of $N/2$.

In the ground state, $\lambda_r \to \infty$ to minimize the energy. The ground state energy in the thermodynamic limit can be easily derived as

$$\begin{aligned}E = {} & -4\pi N\sin\theta\int_{-\infty}^{\infty}a_1(\lambda)\rho(\lambda)d\lambda \\ & - \sin\theta\bigl[4\pi a_k\bigl(\lambda^r\bigr) + \cot(a_+ - \theta/2) + \cot(a_- - \theta/2) - (N-1)\cot\theta\bigr] \\ = {} & Ne_0 + e_b,\end{aligned} \tag{3.15}$$

and

$$e_0 = -\int_{-\infty}^{\infty}\frac{2\sin\theta\sinh^2(\pi\omega/2 - \theta\omega/2)}{\sinh(\pi\omega/2)[\sinh(\pi\omega/2) + \sinh(\pi\omega/2 - \theta\omega)]}d\omega + \cos\theta, \tag{3.16}$$

$$e_b = e_b^0 + I_1(a_+) + I_1(a_-) + 2I_2(\beta) \tag{3.17}$$

with e_0 the ground state energy density of the periodic chain and e_b the surface energy, where

$$e_b^0 = -\sin\theta\int_{-\infty}^{\infty}\frac{\hat{a}_1(\omega)}{1 + \hat{a}_2(\omega)}\bigl[\hat{a}_2(\omega/2) - 1\bigr]d\omega - \cos\theta,$$

$$I_1(\alpha) = \sin\theta\int_{-\infty}^{\infty}\frac{\hat{a}_1(\omega)}{1 + \hat{a}_2(\omega)}\hat{a}_{2\alpha/\theta}(\omega)d\omega - \sin\theta\cot(\alpha - \theta/2),$$

$$I_2(\beta) = -\sin\theta \int_{-\infty}^{\infty} \frac{\hat{a}_1(\omega)}{1+\hat{a}_2(\omega)} \cos(\beta\omega)\hat{b}(\omega)d\omega. \tag{3.18}$$

Some remarks are in order: (1) The extra string in the ground state configuration contributes nothing to the energy in the thermodynamic limit. However, for a finite N, the string may induce exponentially small corrections. (2) Above we considered only the parameter region $a_\pm \in (\pi/2, \pi)$. For the boundary parameters out of this region, stable boundary bound states exist in the ground state [41–44]. However, the energy is indeed a smooth function about the boundary parameters as demonstrated in the diagonal boundary field case [44,45]. (3) An interesting fact is that the contributions of a_+, a_-, β to the energy are completely separated and the surface energy does not depend on $\theta_\pm$ at all (same effect was also obtained in [46] where the surface energy and the finite size correction were derived for some constraint boundary parameters), which indicate that the two boundary fields behave independently in the thermodynamic limit. Similar phenomenon often occurs in the dilute impurity systems. In such a sense, we may adjust $\theta_\pm$ to match $\bar{c} = 0$ for arbitrary η and non-negative integer M_1 without affecting the thermodynamic quantities up to the order of $O(N^{-1})$. We note the surface energy does depend on the relative directions of the boundary fields to the z-axis because of the anisotropy of the bulk. (4) In the above calculations, we put the integral limits to infinity which is reasonable to the surface energy. To account for the finite size corrections of order $1/N$ (Casimir effect or central charge term), one should keep a finite cutoff for the integrals. Calculations can also be performed by the standard finite size correction and Wiener–Hopf methods [47,48,41,42]. The correlations between the two boundaries exist in this order [42,46]. (5) The thermodynamic equations at the degenerate points $\eta = \eta_m$ can also be derived by following the standard method [40]. (6) When $\beta = 0$, the boundary magnetic fields lie in the x–y plane. Taking the limit $\eta \to 0$ of Eq. (3.17) we obtain the surface energy of the XXX spin chain with arbitrary boundary fields, which obviously does not depend on the angles $\theta_\pm$. The $\theta_\pm$-dependence of the ground state energy only occurs in the order of $1/N$ as verified by the numerical simulations [49,50].

Now let us turn to arbitrary $\beta_\pm$ case. In this case, the degenerate points of η takes complex values and the above derivations are invalid. However, we can deduce the surface energy with the following argument. In principle, for $N \to \infty$ the surface energy takes the form

$$\epsilon_b = \epsilon_b^0 + \bar{\epsilon}_b(\alpha_+, \beta_+, \theta_+) + \bar{\epsilon}_b(\alpha_-, \beta_-, \theta_-), \tag{3.19}$$

because the two boundaries decouple completely as long as the bulk is not long-range ordered. Here the second and the third terms are the contributions of the boundary fields. For arbitrary real $\beta_\pm$, suppose

$$\bar{\epsilon}_b(\alpha_\pm, \beta_\pm, \theta_\pm) = I_1(a_\pm) + \bar{I}(a_\pm, \beta_\pm, \theta_\pm). \tag{3.20}$$

When $\beta_\pm = \pm\beta$, from Eqs. (3.17), (3.19), (3.20) we have

$$\bar{I}(a_+, \beta, \theta_+) + \bar{I}(a_-, -\beta, \theta_-) = 2I_2(\beta), \tag{3.21}$$

which indicates that $\bar{I}(\alpha_\pm, \beta_\pm, \theta_\pm)$ does not depend on $\alpha_\pm$ and $\theta_\pm$. In addition, for $\alpha_- = i\pi/2$, the boundary field is an even function of β_-. Since $\bar{I}(\alpha_-, \beta_-, \theta_-)$ is independent of α_-, θ_-, it must be an even function of β_-. The same conclusion holds for β_+. Therefore we conclude that

$$\epsilon_b = \epsilon_b^0 + I_1(a_+) + I_1(a_-) + I_2(\beta_+) + I_2(\beta_-). \tag{3.22}$$

The above formula is valid for arbitrary boundary fields and η in the thermodynamic limit $N \to \infty$ since η_m become dense.

4. Physical quantities for large N and generic η

With the reduced BAEs at the degenerate η points, most of the physical quantities as functions of η_m can be derived up to the order of $1/N$ with the conventional methods, i.e.,

$$F(\eta_m) = Nf_0(\eta_m) + f_1(\mu_m) + \frac{1}{N} f_2(\eta_m) + O\big(N^{-2}\big). \tag{4.1}$$

Let us treat $f_n(\eta)$ $(n = 0, 1, 2)$ as known functions. For a generic $i\eta_m \geq i\eta \geq i\eta_{m+1}$, we suppose that the corresponding quantities are $\bar{f}_n(\eta)$ which are initially unknown functions. We suppose further both $f_n(\eta)$ and $\bar{f}_n(\eta)$ are smooth functions about η. Obviously,

$$\bar{f}_n(\eta_m) = f_n(\eta_m), \tag{4.2}$$

and $\bar{f}_0(\eta) = f_0(\eta)$ because f_0 is boundary-field independent and is the same calculated from the corresponding periodic system. Let us make the following Taylor expansions around η_m and η_{m+1} $(n = 1, 2)$

$$\begin{aligned}
\bar{f}_n(\eta) &= \bar{f}_n(\eta_m) + \bar{f}_n'(\eta_m)\bar{\delta}_1 + O\big(N^{-2}\big) \\
&= f_n(\eta_m) + \bar{f}_n'(\eta_m)\bar{\delta}_1 + O\big(N^{-2}\big) \\
&= f_n(\eta_{m+1}) + \bar{f}_n'(\eta_{m+1})\bar{\delta}_2 + O\big(N^{-2}\big),
\end{aligned} \tag{4.3}$$

with $\bar{\delta}_1 = \eta - \eta_m$ and $\bar{\delta}_2 = \bar{\delta}_1 - \frac{2i\pi}{N}$. Notice that

$$\begin{aligned}
f_n(\eta_{m+1}) &= f_n(\eta_m) + f_n'(\eta_m)\frac{2i\pi}{N} + O\big(N^{-2}\big), \\
f_n'(\eta_{m+1}) &= f_n'(\eta_m) + O\big(N^{-1}\big),
\end{aligned}$$

we readily have

$$\bar{f}_n'(\eta_m) = f_n'(\eta_m) + O\big(N^{-1}\big),$$

and

$$\begin{aligned}
\bar{f}_n(\eta) &= f_n(\eta_m) + f_n'(\eta_m)\bar{\delta}_1 + O\big(N^{-2}\big) \\
&= f_n(\eta) + O\big(N^{-2}\big),
\end{aligned} \tag{4.4}$$

which means that the unknown function $\bar{f}_n(\eta)$ can be replaced by the known function $f_n(\eta)$ up to the order of $O(N^{-2})$.

5. Concluding remarks

In conclusion, a systematic method is proposed for approaching the thermodynamic limit of the ODBA solvable models with the open *XXZ* spin chain as an example. The central idea of this method lies in that at a sequence of degenerate crossing parameter points, the ODBA equations can be reduced to the conventional BAEs, which allows us to derive the thermodynamic quantities with the well developed methods. We remark that there are no degenerate points for the isotropic Heisenberg spin chain model [26], the *XXZ* model for real η and the *XXZ* spin torus [25]. However, the thermodynamic quantities can be observed from their anisotropic correspondences. For the Heisenberg chain, we may take the limit $\eta \to 0$ of the *XXZ* chain, for the *XXZ* chain with real η, we may take a proper limit of *XYZ* model [27], and for the *XXZ* torus, we may take a proper limit of the *XYZ* torus. In fact, for most of the rational integrable models, their trigonometric and elliptic counterparts exist. The latter ones normally possess degenerate points and thus the present method works.

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References

[1] R.J. Baxter, Exactly Solved Models in Statistical Mechanics, Academic Press, London, 1982.
[2] V.E. Korepin, N.M. Bogoliubov, A.G. Izergin, Quantum Inverse Scattering Method and correlation Function, Cambridge University Press, Cambridge, 1993.
[3] A.A. Zvyagin, Finite Size Effects in Correlated Electron Models: Exact Results, Imperial College Press, London, 2005.
[4] T. Giamarchi, Quantum Physics in One Dimension, Oxford University Press, Oxford, 2003.
[5] E.H. Lieb, W. Liniger, Phys. Rev. 130 (1963) 1605.
[6] E.H. Lieb, Phys. Rev. 130 (1963) 1616.
[7] C.N. Yang, Phys. Rev. Lett. 19 (1967) 1312.
[8] E.H. Lieb, F.Y. Wu, Phys. Rev. Lett. 20 (1968) 1445.
[9] X.-W. Guan, M.T. Batchelor, C. Lee, Rev. Mod. Phys. 85 (2013) 1633.
[10] J.A. Minahan, K. Zarembo, J. High Energy Phys. 03 (2003) 013.
[11] N. Beisert, C. Ahn, L.F. Alday, Z. Bajnok, J.M. Drummond, L. Freyhult, N. Gromov, R.A. Janik, V. Kazakov, T. Klose, G.P. Korchemsky, C. Kristjansen, M. Magro, T. McLoughlin, J.A. Minahan, R.I. Nepomechie, A. Rej, R. Roiban, S. Schafer-Nameki, C. Sieg, M. Staudacher, A. Torrielli, A.A. Tseytlin, P. Vieira, D. Volin, K. Zoubos, Lett. Math. Phys. 99 (2012) 1.
[12] D. Berenstein, S.E. Vazquez, J. High Energy Phys. 06 (2005) 059.
[13] D.M. Hofman, J.M. Maldacena, J. High Energy Phys. 11 (2007) 063.
[14] R. Murgan, R.I. Nepomechie, J. High Energy Phys. 09 (2008) 085.
[15] R.I. Nepomechie, J. High Energy Phys. 11 (2011) 069.
[16] J. McGreevy, L. Susskind, N. Toumbas, J. High Energy Phys. 06 (2000) 008.
[17] H. Bethe, Z. Phys. 71 (1931) 205.
[18] F.C. Alcaraz, M.N. Barber, M.T. Batchelor, R.J. Baxter, G.R.W. Quispel, J. Phys. A 20 (1987) 6397.
[19] E.K. Sklyanin, L.D. Faddeev, Sov. Phys. Dokl. 23 (1978) 902.
[20] E.K. Sklyanin, J. Phys. A 21 (1988) 2375.
[21] R.J. Baxter, Phys. Rev. Lett. 26 (1971) 832.
[22] R.J. Baxter, Phys. Rev. Lett. 26 (1971) 834.
[23] L.A. Takhtadzhan, L.D. Faddeev, Russ. Math. Surv. 34 (1979) 11.
[24] C.M. Yung, M.T. Batchelor, Nucl. Phys. B 446 (1995) 461.
[25] J. Cao, W.-L. Yang, K. Shi, Y. Wang, Phys. Rev. Lett. 111 (2013) 137201.
[26] J. Cao, W.-L. Yang, K. Shi, Y. Wang, Nucl. Phys. B 875 (2013) 152.
[27] J. Cao, W.-L. Yang, K. Shi, Y. Wang, Nucl. Phys. B 877 (2013) 152.
[28] R.I. Nepomechie, Nucl. Phys. B 622 (2002) 615.
[29] R.I. Nepomechie, J. Phys. A 37 (2004) 433.
[30] A.M. Povolotsky, Phys. Rev. E 69 (2004) 061109.
[31] J. de Gier, F.H.L. Essler, Phys. Rev. Lett. 95 (2005) 240601.
[32] A.M. Povolotsky, J.F.F. Mendes, J. Stat. Phys. 123 (2006) 125.

[33] C. Winkelholz, R. Fazio, F.W.J. Hekking, G. Schön, Phys. Rev. Lett. 77 (1996) 3200.
[34] Y.-Y. Li, J. Cao, W.-L. Yang, K. Shi, Y. Wang, Nucl. Phys. B 879 (2014) 98.
[35] R.I. Nepomechie, J. Phys. A 46 (2013) 442002.
[36] J. Cao, W.-L. Yang, K. Shi, Y. Wang, arXiv:1307.0280.
[37] X. Zhang, J. Cao, W.-L. Yang, K. Shi, Y. Wang, arXiv:1312.0376.
[38] J. Cao, K. Shi, H.-Q. Lin, Y. Wang, Nucl. Phys. B 663 (2003) 487.
[39] R.I. Nepomechie, F. Ravanini, J. Phys. A 36 (2003) 11391.
[40] M. Takahashi, Thermodynamics of One-Dimensional Solvable Models, Cambridge University Press, Cambridge, 1999.
[41] C.J. Hamer, G.R.W. Quispel, M.T. Batchelor, J. Phys. A 20 (1987) 5677.
[42] M.T. Batchelor, C.J. Hamer, J. Phys. A 23 (1990) 761.
[43] S. Skorik, H. Saleur, J. Phys. A 28 (1995) 6605.
[44] A. Kapustin, S. Skorik, J. Phys. A 29 (1996) 1629.
[45] R. Murgan, R.I. Nepomechie, C. Shi, J. High Energy Phys. 01 (2007) 038.
[46] C. Ahn, R.I. Nepomechie, Nucl. Phys. B 676 (2004) 637.
[47] C.N. Yang, C.P. Yang, Phys. Rev. 150 (1966) 327.
[48] H.J. de Vega, F. Woynarowich, Nucl. Phys. B 251 (1985) 439.
[49] Y. Jiang, S. Cui, J. Cao, W.-L. Yang, K. Shi, Y. Wang, arXiv:1309.6456.
[50] R.I. Nepomechie, C. Wang, J. Phys. A 47 (2014) 079501.